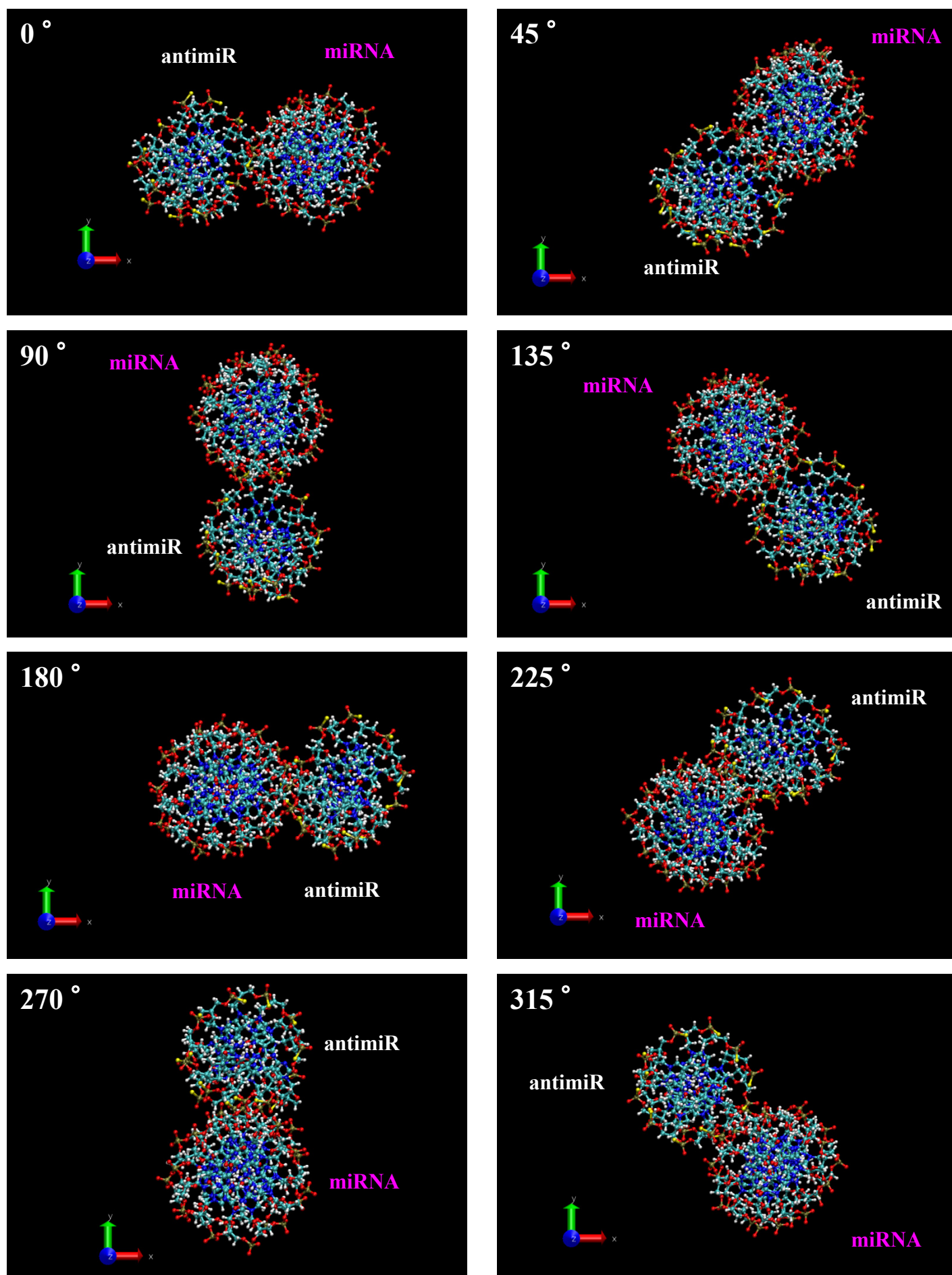
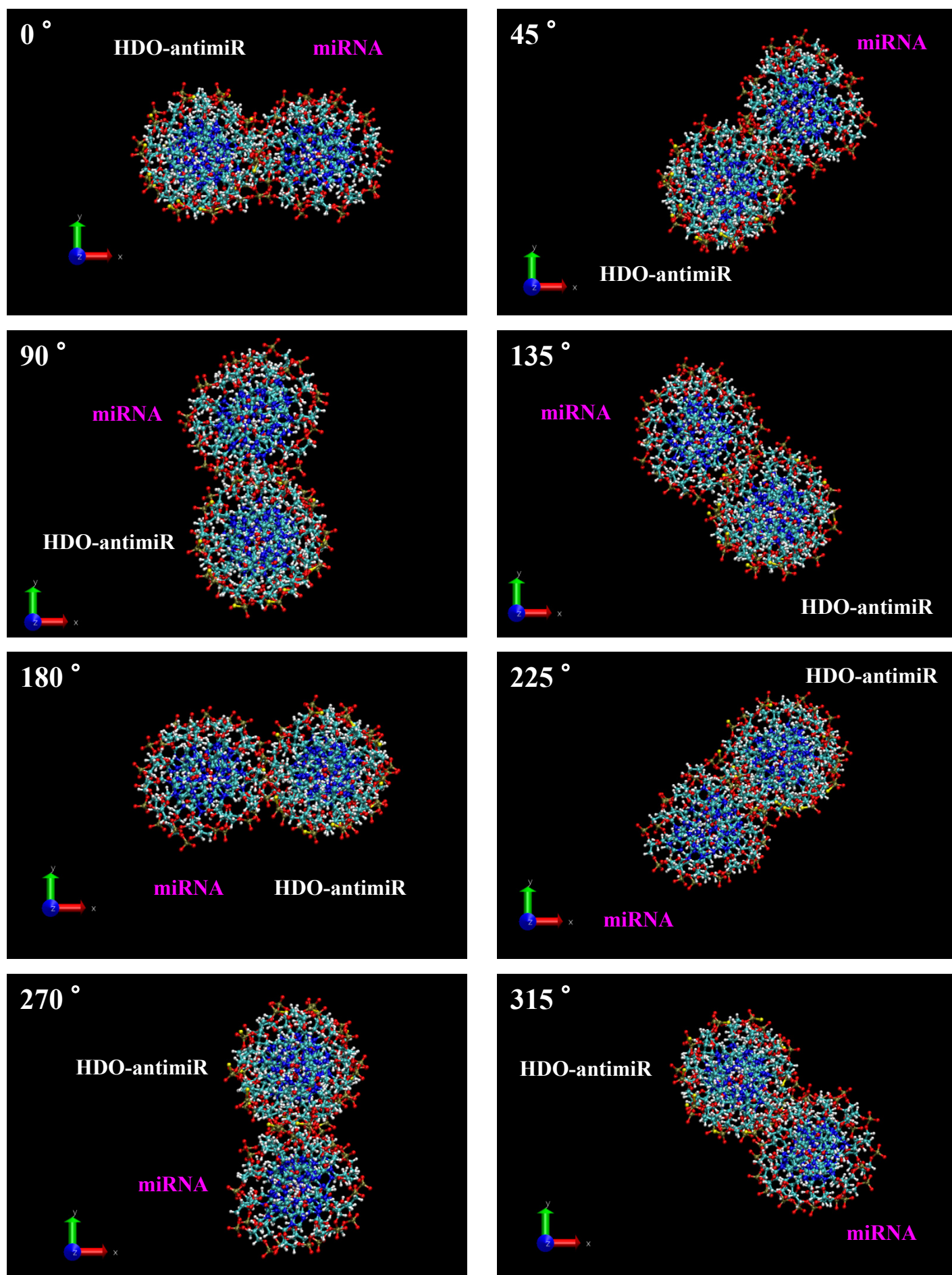


Supplementary Figure 1



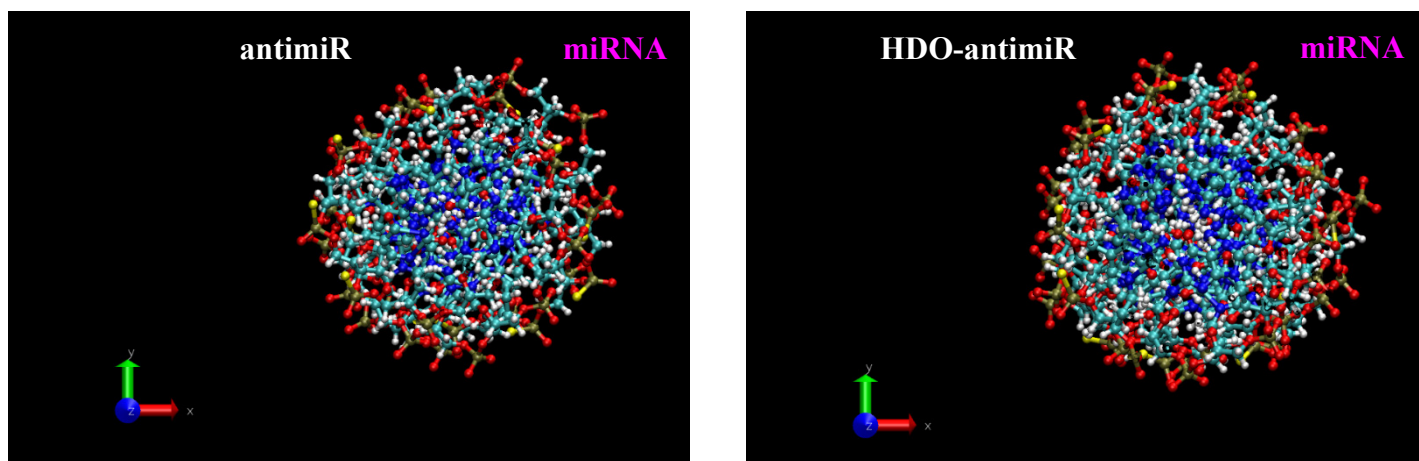
Initial structure of anti-miR122 and miR122. White: H, Red: O, Light blue: C, Blue: N, Gold: P, Yellow: S

Supplementary Figure 2



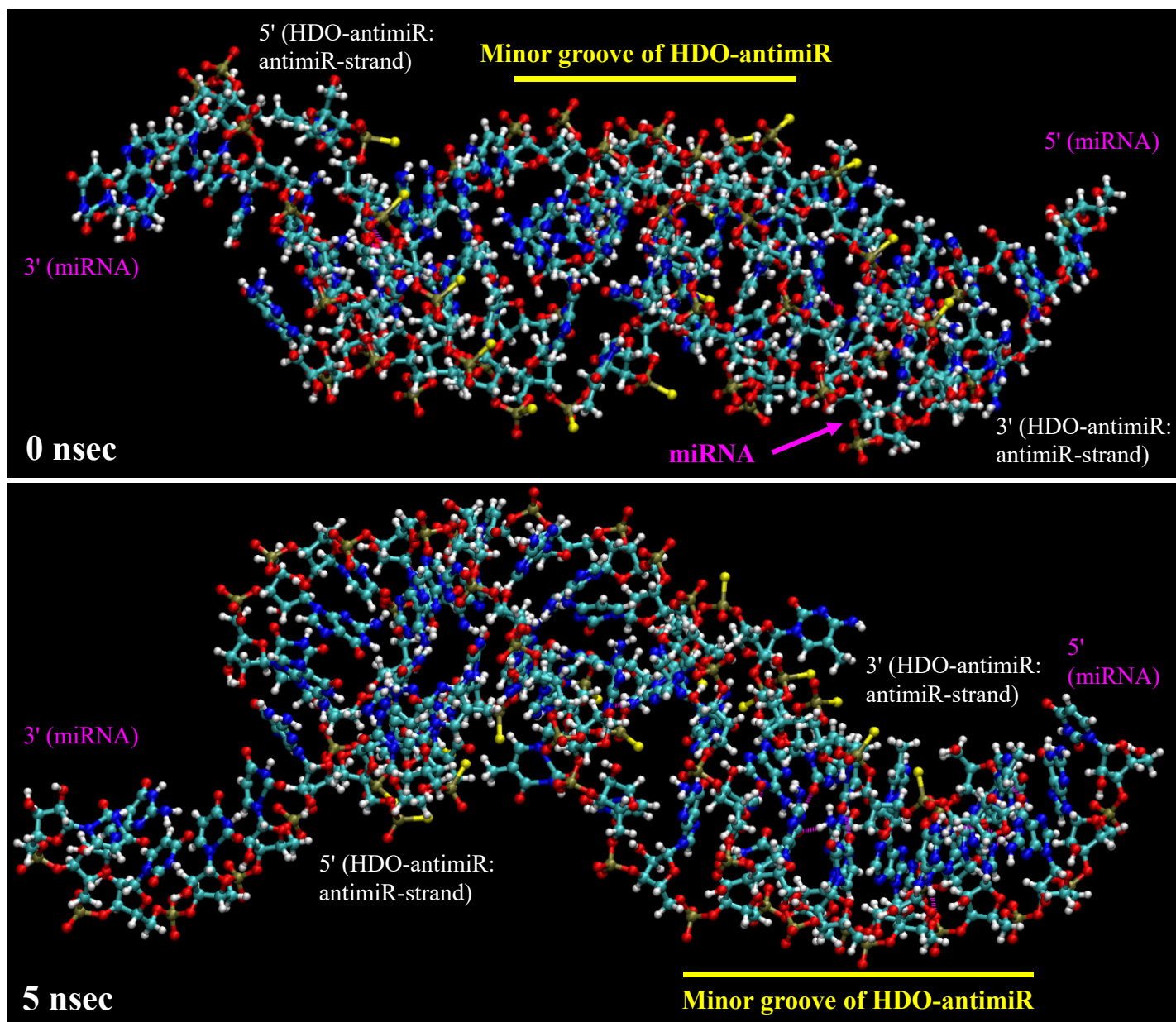
Initial structure of HDO-antimiR122 and miR122. White: H, Red: O, Light blue: C, Blue: N, Gold: P, Yellow: S

Supplementary Figure 3



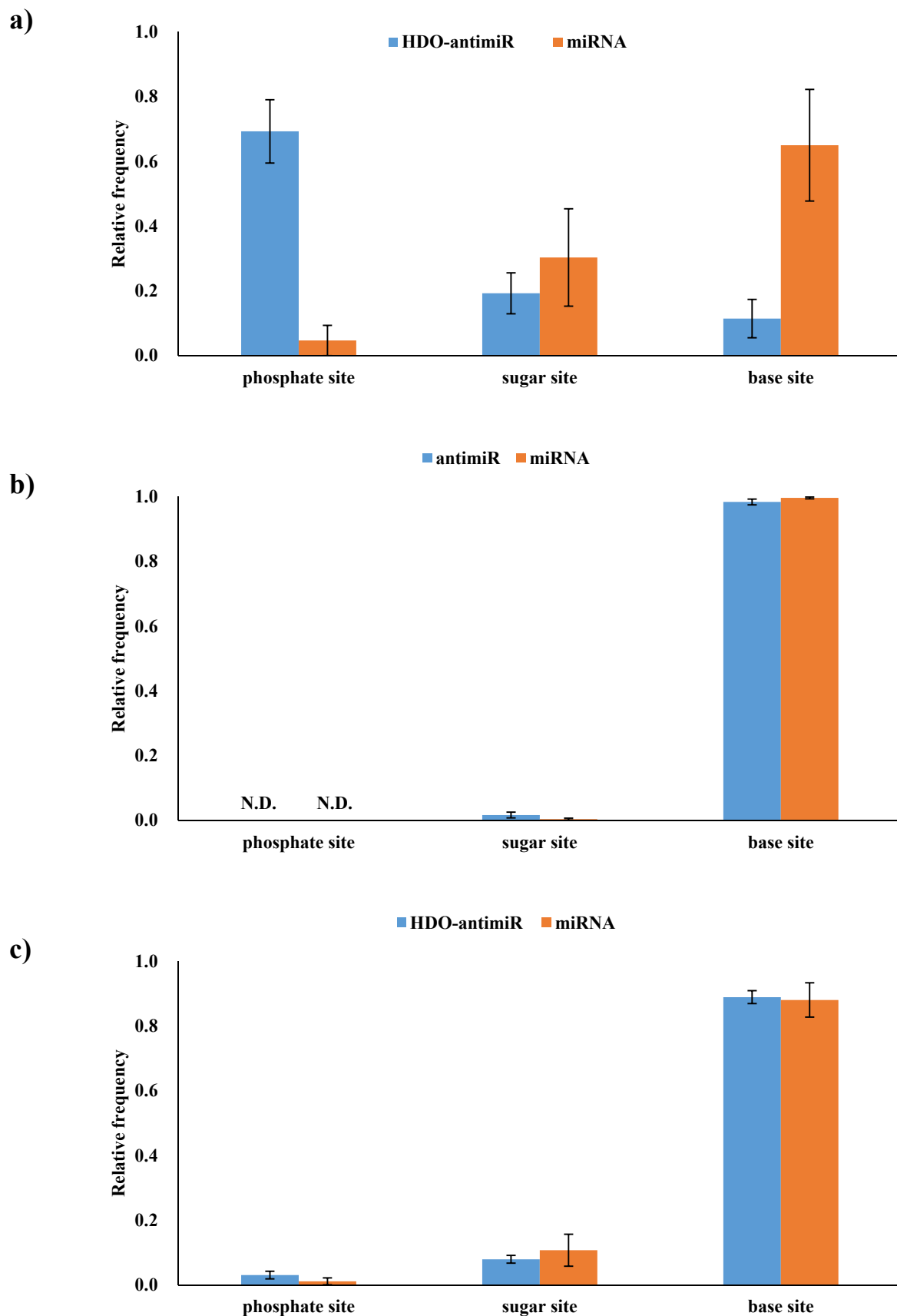
Shift anti-miR122 or HDO-anti-miR122 -5 Å from miR122 in the sagittal direction, initial structure.
White: H, Red: O, Light blue: C, Blue: N, Gold: P, Yellow: S

Supplementary Figure 4



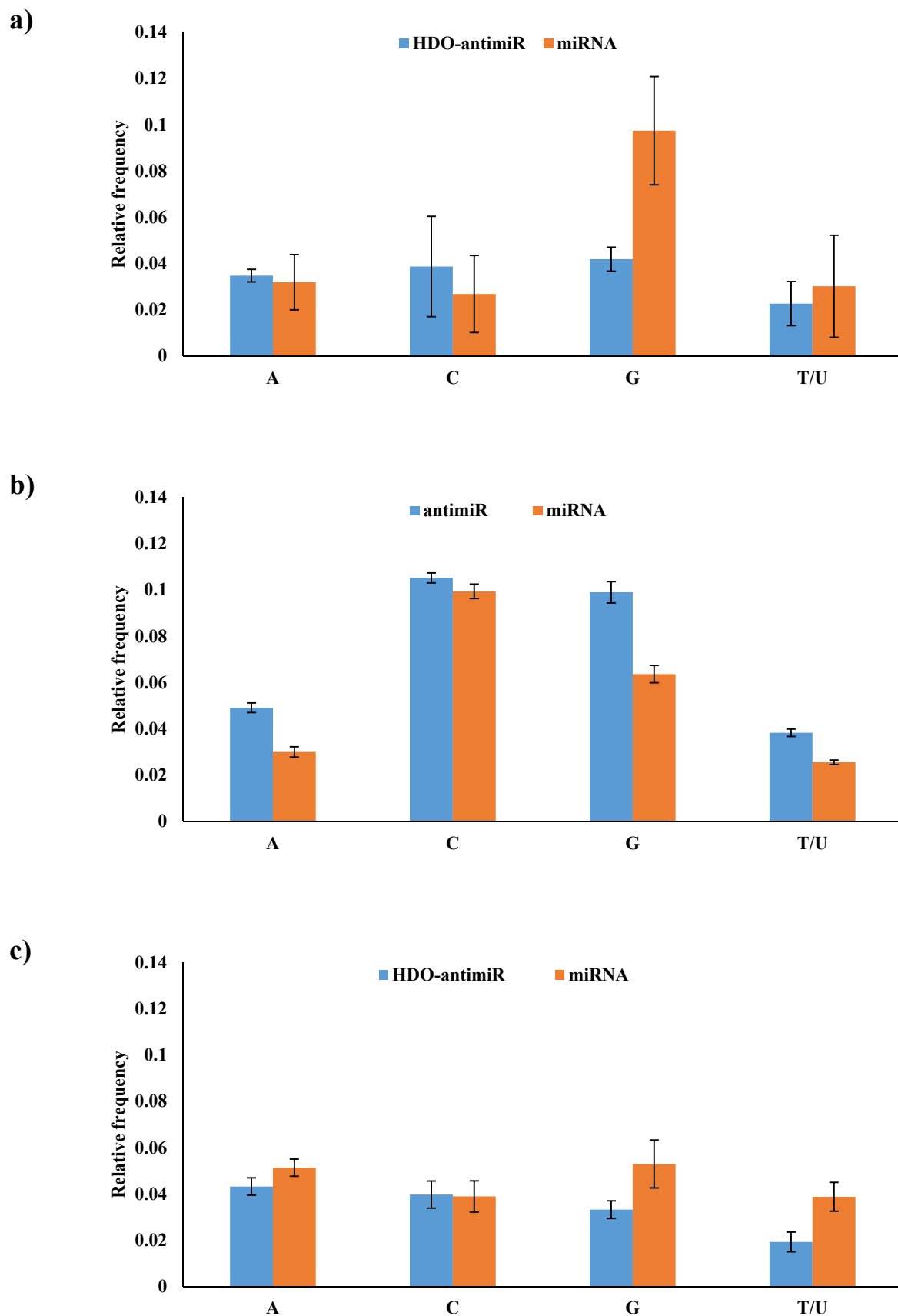
Shift HDO-anti-miR122 +5 Å from miR122 in the sagittal direction. White: H, Red: O, Light blue: C, Blue: N, Gold: P, Yellow: S, Magenta: Hydrogen bond between HDO-anti-miR and miRNA
(The hydrogen bonds are indicated by dashed lines)

Supplementary Figure 5



Analyses about binding site of the number of hydrogen bonds between anti-miR21 or HDO-anti-miR21 and miR21. a) HDO-anti-miR21; 20 Å shifted from miR21 in the horizontal section, Two-point interaction pattern. The results are presented as mean $\pm$ SEM (n = 3). b) anti-miR21; -5 Å shifted from miR21 in the sagittal direction. The results are presented as mean $\pm$ SEM (n = 3). N.D., not detected. c) HDO-anti-miR21; -5 Å shifted from miR21 in the sagittal direction. The results are presented as mean $\pm$ SEM (n = 3).

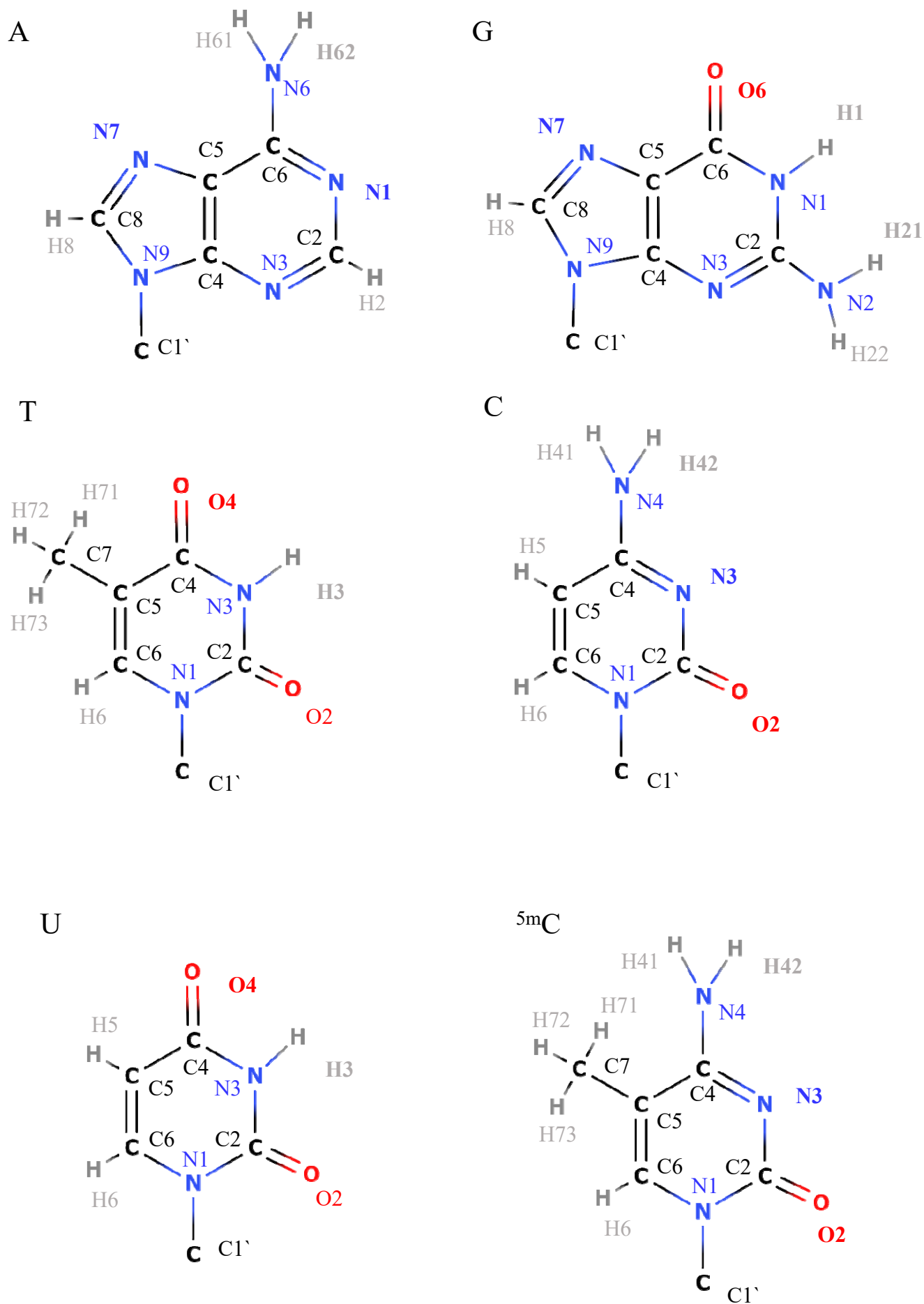
Supplementary Figure 6



Analyses about base site of the number of hydrogen bonds between antimiR21 or HDO-antimiR21 and miR21. a) HDO-antimiR21; 20 Å shifted from miR21 in the horizontal section, Two-point interaction pattern. The results are presented as mean $\pm$ SEM (n = 3). b) antimiR21; -5 Å shifted from miR21 in the sagittal direction. The results are presented as mean $\pm$ SEM (n = 3). c) HDO-antimiR21; -5 Å shifted from miR21 in the sagittal direction. The results are presented as mean $\pm$ SEM (n = 3).

Supplementary Figure 7

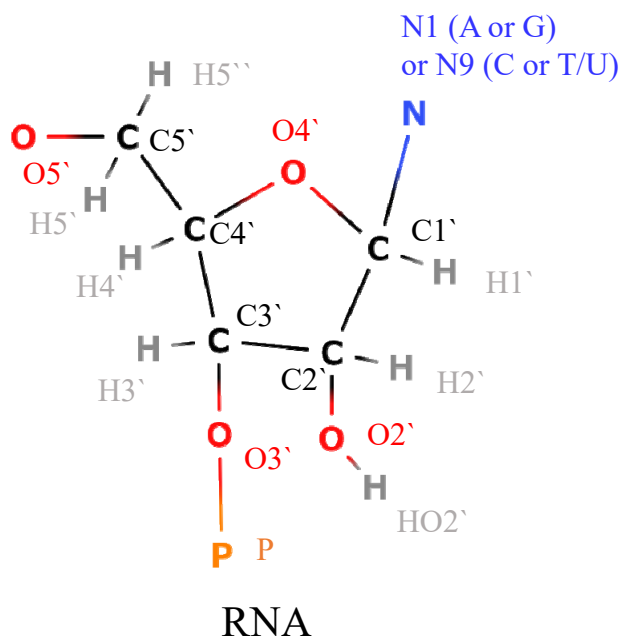
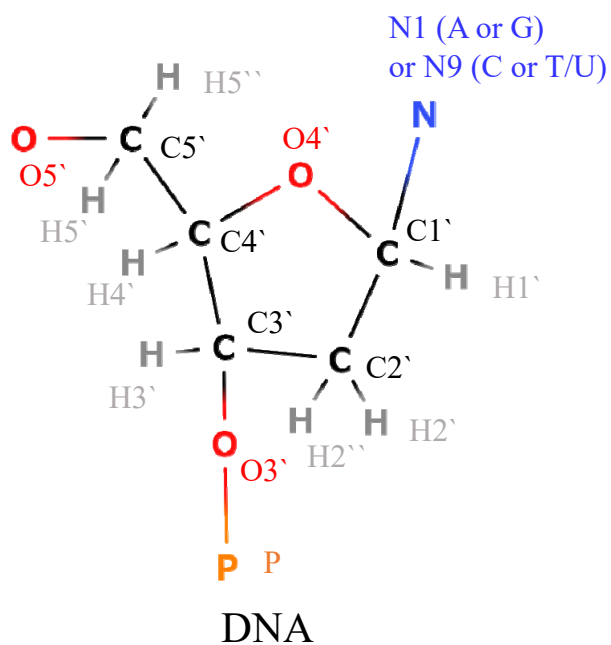
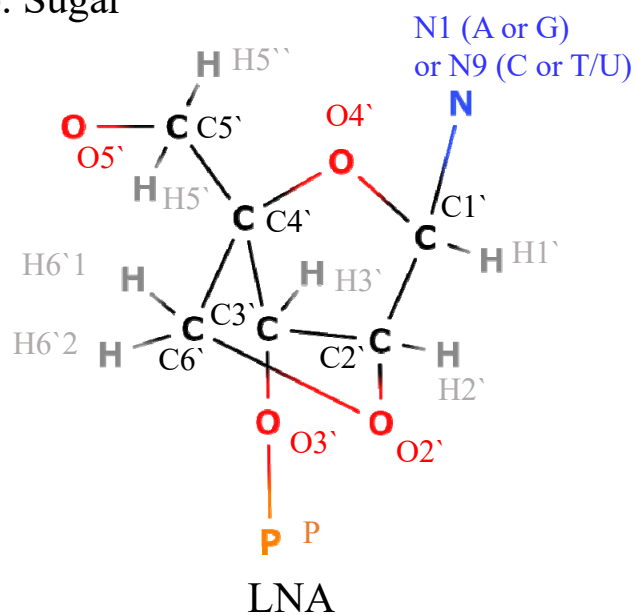
a. Base



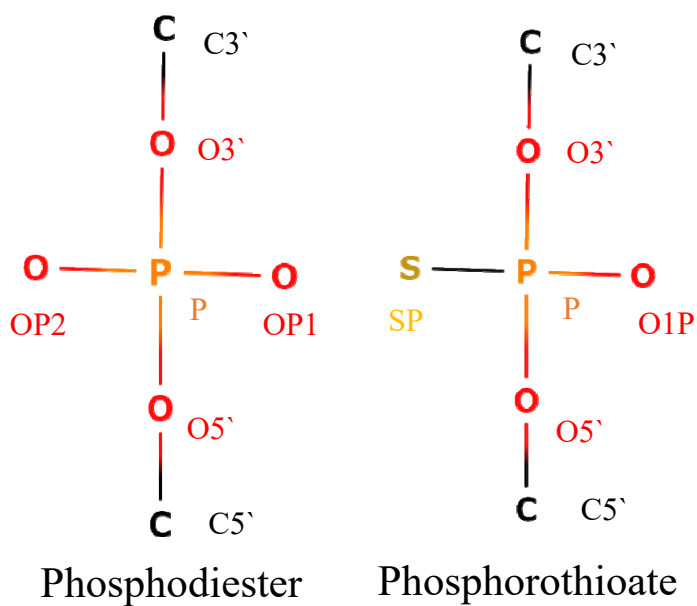
Atoms of each oligonucleotide with index.

Supplementary Figure 7 (cont.)

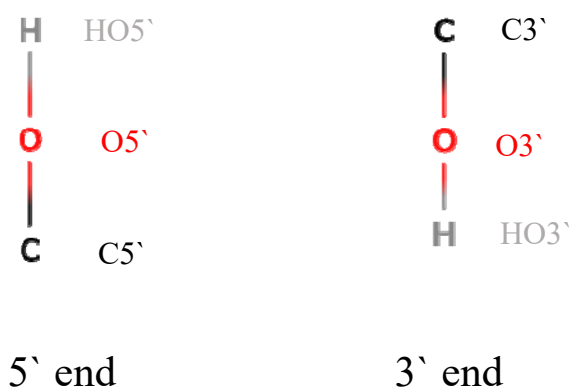
b. Sugar



c. Phosphate linkage



d. End of the oligonucleotide



Atoms of each oligonucleotide with index.

Supplementary Table 1

Multiple-point 1			Two-point 1			Two-point 2			Two-point 3		
antimiR	miRNA	freq.	antimiR	miRNA	freq.	antimiR	miRNA	freq.	antimiR	miRNA	freq.
DA9 O1P	G24 N2	23.06%	DC8 N4	A28 OP2	12.64%	LA3 N6	G33 N3	9.36%	LC1 O5'	G33 O2'	4.36%
LA3 O3'	G33 N2	19.24%	LC15 O3'	G17 OP2	8.32%	LA3 N1	G33 N2	9.08%	LC15 N4	G22 N3	3.92%
DC8 N4	A25 OP1	13.94%	DA9 N6	A27 OP1	4.88%	DT4 O2	G33 N2	8.44%	DA11 N6	G24 OP1	2.40%
DT5 O1P	G31 N1	6.84%	LA3 O1P	G37 N2	4.16%	DT4 N3	U34 O4	4.34%	LC12 N4	G24 OP1	2.18%
DT5 O1P	G30 N2	4.94%	LC15 O3'	G17 OP1	3.44%	DC2 N4	U32 O2'	3.74%	LC15 N4	U21 O2	2.12%
DT4 O1P	G33 N2	4.24%	DC2 O3'	G37 N2	3.26%	LA3 N6	U32 O2'	2.88%	LC15 N4	U21 O2'	1.82%
DC2 N4	U36 O2'	4.12%	LC10 N4	C26 O2	2.34%	LA3 N3	G31 N2	2.60%	LC1 N3	G33 N2	1.52%
DT5 O1P	G31 N2	3.36%	LC1 O2	U38 O3'	2.30%	LA3 O2'	G31 N2	1.64%	DC2 N4	U34 OP1	1.46%
LA3 O2'	G33 N1	2.44%	LC1 N4	U38 O3'	1.72%	LC15 N4	G22 N3	1.54%	LC1 N4	G33 N3	1.34%
DT4 O3'	G31 N1	2.18%	DC2 N4	G37 O6	1.60%	LA3 N1	U32 N3	0.96%	DT13 N3	U23 O2	1.04%
DC2 N4	G37 N3	2.14%	DC2 O2	G37 N2	1.56%	DC2 N4	U32 O2	0.92%	LC14 O2	U23 N3	0.76%
DT4 O1P	U32 N3	1.98%	DC2 N3	G37 N1	1.16%	DC2 N4	G33 OP1	0.62%	LC1 O2'	G33 N2	0.72%
DC2 N4	U38 O4	1.86%	DC2 N4	U38 O2'	1.14%	LA3 O2'	G30 N1	0.60%	LC15 N4	U21 O4	0.66%
DC8 O2	G24 N2	1.74%	DC2 N4	G37 N1	1.00%	LC1 N4	G33 OP1	0.52%	LC15 N3	G22 N2	0.56%
DT5 O1P	G30 N1	1.66%	DC8 N4	A28 OP1	0.96%	LC15 C5	G22 N2	0.50%	LC15 O2	G22 N2	0.54%
LA3 O3'	G33 N1	1.42%	LC1 N3	U38 O3'	0.76%	LC15 N3	G22 N2	0.50%	LC15 N3	U21 N3	0.50%
LC1 O2'	G37 N2	1.24%	DC2 N4	U35 O2	0.74%	DC2 N4	U32 O4'	0.48%	LC1 O2	G33 O2'	0.44%
DC2 N4	G37 N2	0.92%	DA9 N6	C26 O3'	0.72%	LC1 N4	U32 O2'	0.38%	LC10 N4	A25 OP1	0.44%
DC2 O2	U36 N3	0.92%	LA3 O1P	U36 N3	0.70%	DT5 O1P	A28 N6	0.32%	LC1 O2	G33 N2	0.40%
LA3 N1	G37 N2	0.40%	DC2 N4	U38 O4	0.68%	LC15 N4	U21 O2'	0.32%	LC1 N4	G33 N2	0.32%
LC1 O3'	G37 N2	0.38%	DC2 O2	U35 N3	0.54%	LA3 O2'	G30 N2	0.30%	LC15 N4	U21 N3	0.30%
DC2 N3	U36 N3	0.34%	DA9 N6	C26 O2	0.46%	LC1 N4	U32 O3'	0.30%	LC1 N4	U34 O2	0.28%
DC2 N3	G37 N2	0.18%	DC2 N4	U36 N3	0.44%	DT5 O2	G33 N2	0.26%	DC2 N4	G33 O3'	0.18%
DT4 O3'	G31 N2	0.14%	DC2 O3'	U38 O2'	0.44%	LA3 N6	U32 O2	0.16%	LC15 N4	U23 O4	0.18%
DT4 O1P	G33 N1	0.14%	DA11 N1	C26 N4	0.40%	LC15 O2'	G20 N2	0.12%	LC15 O2	U21 N3	0.14%
LA3 N3	U36 N3	0.14%	LC15 O3'	G18 OP2	0.38%						
LC1 O5'	U38 O4	0.14%	DC2 O2	U38 O2'	0.36%						
LC1 O5'	G37 N2	0.12%	DA11 N6	C26 N3	0.34%						
			DC2 N4	U36 O4	0.34%						
			DC2 N3	G37 N2	0.30%						
			DA11 N6	C26 O2	0.24%						
			DC2 O4'	G37 N2	0.24%						
			LA3 O1P	G37 N1	0.22%						
			DC2 O2	G37 N1	0.22%						
			LC1 O2'	U38 O3'	0.22%						
			DC2 O2	U36 N3	0.16%						
			LC1 O2'	U38 O2'	0.12%						

The frequency of the binding site of the antimiR122 with miR122.
(Multiple-point and Two-point interaction pattern, more than 0.1% frequency)

Supplementary Table 2

Multiple-point 1			Multiple-point 2			Multiple-point 3			Multiple-point 4		
HDO	miRNA	freq.	HDO	miRNA	freq.	HDO	miRNA	freq.	HDO	miRNA	freq.
U22 OP1	G37 N2	19.62%	G19 OP1	G37 N2	14.72%	G17 OP1	G33 N1	13.18%	G30 O3'	U51 OP1	6.66%
U22 OP1	U38 N3	6.38%	LC15 O2'	G33 N1	11.24%	G16 O3'	G32 N1	9.52%	LC15 O2'	G32 N1	6.00%
G23 OP1	G39 N2	5.22%	G19 OP2	G37 N1	9.00%	G19 OP1	G37 N2	5.34%	G19 OP1	G39 N2	4.62%
LC1 O5'	C41 OP1	3.58%	LC15 O2'	G33 N2	5.08%	U20 OP1	G37 N2	5.08%	U20 OP1	G39 N1	4.44%
U22 OP2	G39 N1	2.32%	U20 OP1	G37 N2	4.22%	G17 OP1	G33 N2	3.76%	U20 OP1	G39 N2	4.34%
G21 O3'	G37 N1	2.06%	LC15 O3'	G33 N2	3.84%	G19 OP1	G35 N2	3.70%	LC15 N3	G33 N2	4.30%
LC14 O1P	G35 N2	1.68%	G17 O2'	G35 O6	2.76%	U20 OP2	G37 N1	3.68%	G19 OP2	A40 N6	4.20%
DT13 O1P	G33 N2	1.66%	G16 N2	G32 OP1	2.68%	G16 O2'	U31 O4	2.82%	U20 OP2	G39 N2	3.76%
U22 OP1	G39 N1	1.44%	LC15 O2'	G32 N1	2.30%	G19 OP1	U38 O2'	2.64%	LC15 O2'	G33 N2	3.26%
DT13 O3'	G35 N2	1.36%	LC15 O3'	G32 N2	2.22%	G17 OP1	G32 N1	2.62%	LC15 O3'	G32 N2	3.00%
U22 OP1	G39 N2	0.92%	G16 N2	G32 OP2	2.08%	G17 OP1	G32 N2	2.36%	LC15 N4	G33 N3	2.44%
DA3 O1P	C41 O2'	0.90%	G17 O2'	A34 N6	1.76%	A18 OP1	G35 N1	2.22%	G30 O2'	U51 OP1	2.12%
U22 OP2	G37 N2	0.88%	LC15 O3'	U31 O4	1.52%	G16 O2'	G32 N2	1.80%	G19 OP1	A40 N6	1.82%
LC14 O1P	G35 N1	0.64%	G19 OP1	G37 N1	1.50%	G19 OP2	G35 N2	1.62%	U20 OP1	U38 N3	1.34%
U22 OP2	G37 N1	0.62%	G16 N2	A34 N1	1.40%	A18 OP1	G35 N2	1.56%	G19 OP2	G39 N2	0.80%
DT13 O3'	A34 N6	0.60%	LC15 O3'	G32 O6	1.18%	G16 O3'	G32 N2	0.92%	LC15 N4	G32 N2	0.78%
U22 OP1	G37 N1	0.60%	LC15 O3'	G32 N1	1.16%	A18 OP1	G37 N2	0.74%	G30 O3'	U50 O3'	0.70%
LC14 O1P	A34 N6	0.52%	LC15 O2'	G32 N2	0.56%	G19 OP1	U36 N3	0.54%	G17 O2'	U31 O4	0.64%
LC15 O1P	G32 O2'	0.48%	G17 O2'	G33 OP2	0.56%	A18 OP2	G33 N2	0.52%	G19 OP1	G39 N1	0.64%
LC1 N4	A40 O2'	0.32%	U20 OP2	G39 N2	0.54%	A18 O3'	G37 N2	0.46%	U20 OP2	G39 N1	0.64%
LC1 O2	G39 N2	0.12%	G19 OP1	G39 N2	0.48%	G19 OP2	G35 N1	0.44%	LC15 O2'	G32 N2	0.52%
G23 OP2	G39 N2	0.12%	G16 N2	G33 N1	0.40%	G16 O5'	U31 O4	0.42%	A18 OP1	A40 N6	0.42%
			U20 OP1	G37 N1	0.34%	G19 OP1	G37 N1	0.40%	G16 N2	U31 O4	0.38%
			U20 OP2	G37 N2	0.30%	G16 O3'	G33 N2	0.38%	LC15 N3	G32 N2	0.34%
			G19 OP2	G37 N2	0.24%	G19 O3'	G37 N1	0.34%	G19 OP2	G39 N1	0.30%
			G19 OP1	G39 N1	0.24%	A18 OP1	A34 N6	0.30%	A18 O3'	G39 N1	0.28%
			G16 N3	A34 N6	0.14%	A18 OP1	G33 N2	0.30%	G17 O2'	G33 N2	0.20%
			LC15 O3'	G33 N1	0.14%	A18 O2'	G37 N2	0.30%	LC15 O3'	G33 N2	0.18%
			G16 N2	G33 O6	0.14%	U20 OP2	G37 N2	0.30%	A18 O2'	U38 N3	0.16%
Multiple-point 5						G19 OP1	U38 N3	0.30%			
HDO	miRNA	freq.				U20 OP1	U38 N3	0.26%			
DT13 O1P	G35 N1	14.92%				DT5 O1P	G39 N2	0.18%			
G21 OP1	U38 O2'	14.16%				U20 OP1	G37 N1	0.16%			
LC12 O3'	G35 N2	11.16%				A18 O3'	U38 N3	0.16%			
LC12 O2'	G37 N2	2.46%				A18 OP1	G33 N1	0.12%			
DT13 O1P	A34 N6	2.16%									
LA3 O1P	A42 N6	1.80%									
U20 O2'	U38 O2	1.72%									
LC12 O2'	G37 N1	1.44%									
DT13 O1P	G35 N2	1.12%									
U20 O2'	G37 O2'	0.68%									
LC12 O2'	U36 N3	0.56%									
U20 O4'	G37 N2	0.54%									
LC12 O2	G37 N2	0.28%									
DC2 O3'	A42 N6	0.26%									
LC12 O2'	G35 N2	0.18%									
U20 O2	G37 N2	0.18%									
LC12 O1P	A34 N6	0.16%									
LC14 O1P	A34 O2'	0.12%									

The frequency of the binding site of the HDO-antimiR122 with miR122.
(Multiple-point interaction pattern, more than 0.1% frequency)

Supplementary Table 3

Two-point 1			Two-point 2		
antimiR	miRNA	freq.	antimiR	miRNA	freq.
LT15 O3'	A17 OP2	14.42%	DG8 N2	U29 OP1	26.76%
DC2 O2	A37 O2'	13.08%	DG8 N1	C28 O3'	16.14%
LT15 O4	U16 N3	6.44%	LT10 O2	G26 N2	14.64%
LT15 N3	U16 O4	4.10%	LC14 O1P	A17 N6	4.22%
LC14 O2	G18 N1	3.78%	LT10 O2'	G26 N2	2.80%
LC14 O2'	G18 N2	3.26%	DC2 O1P	A31 N6	1.52%
DC2 N3	A37 O2'	3.10%	DG8 N1	U29 OP1	0.76%
LC14 O2'	A17 N6	2.62%	LC14 O1P	C19 N4	0.56%
LT15 O3'	A17 N6	2.02%	LT10 O3'	G26 N2	0.56%
LC14 O2'	G18 N1	1.86%	DG13 O3'	A17 N6	0.52%
LC14 O2	A17 N6	1.22%	DG8 N2	U29 OP2	0.48%
LT15 O1P	A17 N6	1.18%	DA11 O1P	G26 N2	0.44%
DC2 N4	A37 O2'	1.14%	DG8 O6	C28 O2'	0.22%
LT1 O2	A37 O3'	0.96%	DG8 N2	C28 O3'	0.18%
DC2 N4	A37 O3'	0.76%			
DC2 N4	A37 N7	0.38%			
LC14 O2	G18 N2	0.36%			
LT15 O3'	A17 N7	0.28%			
LT15 O2	A17 N6	0.26%			
DG13 N2	G18 O6	0.20%			
LT1 N3	A37 O2'	0.16%			
LT15 O1P	U16 N3	0.12%			

Two-point 1			Two-point 2			Two-point 3		
HDO	miRNA	freq.	HDO	miRNA	freq.	HDO	miRNA	freq.
LC14 O1P	G33 O2'	20.26%	U20 OP1	U31 O5'	11.70%	LT10 O1P	G41 N2	21.68%
DG13 O1P	G33 N2	7.84%	G48 N2	A30 OP1	8.54%	G25 OP1	U44 N3	10.94%
DC2 O1P	A46 N6	5.34%	C18 O2'	U31 O5'	7.40%	A26 OP2	G45 N2	10.82%
LA12 O1P	A32 N6	4.16%	A30 OP1	U47 N3	5.36%	A24 O3'	C43 N4	9.62%
LC14 O1P	C34 N4	4.12%	U19 OP1	U31 O5'	4.68%	G25 OP1	G45 N2	8.30%
LA12 O3'	G33 N2	3.46%	A30 OP2	G48 N2	4.00%	G25 OP1	G45 N1	3.22%
A30 OP1	A52 O3'	2.84%	A30 OP1	G48 N1	3.42%	A26 OP2	A46 N6	2.80%
G29 N2	A52 O2'	2.62%	DG13 N2	U31 O4	3.18%	C23 O2'	G41 N1	2.28%
A30 N6	A52 O2'	2.60%	G29 O3'	G48 N1	3.08%	LA12 O1P	C34 N4	1.66%
LA12 O1P	G33 N2	2.54%	A30 O2'	G45 N1	2.72%	A24 OP1	A42 N6	1.46%
LC14 O1P	G33 N2	2.42%	LC14 O2'	U31 N3	0.98%	G25 OP1	C43 N4	1.32%
DG13 O1P	G33 N1	1.04%	U19 OP1	A32 N6	0.88%	LA12 O1P	A40 N6	0.96%
A30 N7	A52 O2'	0.94%	A30 O3'	G45 N2	0.86%	C23 O2'	G41 N2	0.64%
G29 O2'	A52 O3'	0.92%	A30 O2'	G45 O6	0.36%	C23 O3'	A42 N6	0.62%
LT15 O1P	G33 O2'	0.92%	LT15 O3'	U31 O2'	0.36%	DG13 O1P	C34 O2'	0.52%
A30 OP1	A52 O2'	0.76%	A30 O3'	G45 N2	0.34%	C23 O3'	G41 N1	0.44%
U22 OP1	G41 N2	0.64%	A30 O3'	U47 O2	0.30%	LT10 O5'	G41 N2	0.34%
LT15 O1P	C34 N4	0.56%	C18 O3'	A32 N6	0.30%	A24 O2'	C43 N4	0.32%
DG13 O1P	A32 N6	0.36%	A30 O2'	G45 N2	0.28%	A26 OP1	A46 N6	0.28%
LC14 O1P	G33 N1	0.36%	C18 O2'	U31 O2	0.28%	A24 O5'	A42 N6	0.20%
G29 O2'	A52 O2'	0.34%	A30 O3'	G45 N1	0.26%	LT10 O2'	A40 N6	0.16%
A30 N7	A52 O3'	0.34%	U20 OP1	U31 N3	0.26%	A24 O2'	C43 N3	0.14%
LA12 O2'	G33 N2	0.32%	LC14 O2	U31 O2'	0.20%	DG13 O1P	G33 N2	0.12%
LA12 O1P	G33 N1	0.30%	C18 O3'	U31 O5'	0.16%			
G29 O3'	A52 O2'	0.28%	C18 O2'	U31 O5'	0.14%			
LA12 O3'	G33 N1	0.28%						
A30 N6	A52 O3'	0.14%						
LA3 O1P	G51 N2	0.12%						

The frequency of the binding site of the antimiR21 or HDO-antimiR21 with miR21.
(Two-point interaction pattern, more than 0.1% frequency)

Supplementary Table 4

antimiR 1			antimiR 2			antimiR 3		
antimiR	miRNA	freq.	antimiR	miRNA	freq.	antimiR	miRNA	freq.
DC2 O2	G30 N2	53.74%	DC2 O2	G30 N2	51.80%	LC10 O2	G22 N2	48.06%
DC2 N4	G30 O6	42.92%	DC2 N4	G30 O6	45.76%	DC8 N4	G24 O6	42.40%
DC2 N3	G30 N1	40.94%	LC10 O2	G22 N2	44.80%	DC2 O2	G30 N2	38.28%
DC8 O2	G24 N2	39.56%	LG6 O6	C26 N4	43.88%	DC8 O2	G24 N2	37.98%
LC1 O2	G31 N2	36.76%	DC2 N3	G30 N1	40.32%	DA11 N6	U21 O4	37.00%
DT5 O4	A27 N6	33.76%	LG6 N2	C26 O2	38.92%	LC10 N3	G22 N1	35.96%
DC8 N4	G24 O6	33.48%	DC8 O2	G24 N2	38.64%	DC2 N4	G30 O6	35.60%
DC8 N3	G24 N1	31.90%	LG6 N1	C26 N3	36.94%	DC2 N3	G30 N1	33.74%
LA3 N6	U29 O4	31.88%	DC8 N4	G24 O6	36.80%	LC12 O2	G20 N2	33.24%
DT4 O4	A28 N6	27.60%	LC10 N3	G22 N1	35.16%	LC14 O2	G18 N2	31.72%
LC10 O2	G22 N2	25.74%	LA3 N6	U29 O4	31.86%	DT5 O4	A27 N6	31.62%
LC12 O2	G20 N2	25.18%	LC1 O2	G31 N2	30.54%	DA9 N1	U23 N3	28.92%
DA9 N6	U23 O4	24.38%	DA9 N6	U23 O4	29.48%	DC8 N3	G24 N1	28.74%
LC1 N3	G31 N1	23.06%	DC8 N3	G24 N1	28.10%	LC14 N3	G18 N1	26.68%
LG6 N1	C26 O2	22.96%	DA9 N1	U23 N3	27.80%	LC12 N3	G20 N1	26.20%
DT4 N3	A28 N1	21.14%	LT7 N3	A25 N1	27.52%	LC12 N4	G20 O6	25.54%
LA3 N1	U29 N3	20.76%	LC1 N3	G31 N1	27.08%	LC10 N4	G22 O6	25.28%
LC14 O2	G18 N2	19.54%	LC10 N4	G22 O6	23.74%	DA9 N6	U23 O4	24.92%
LC12 N3	G20 N1	18.66%	DT4 O4	A28 N6	22.36%	LG6 O6	C26 N4	24.20%
LC1 N4	G31 O6	17.32%	DT5 O2	A27 N6	17.20%	LG6 N2	C26 O2	23.70%
DA11 N6	G20 O6	15.74%	LC12 O2	G20 N2	16.42%	LC14 N4	G18 O6	23.44%
DA9 N1	U23 N3	14.86%	LA3 N1	U29 N3	15.08%	DA11 N1	U21 N3	23.10%
LT7 O4	A25 N6	14.48%	LC1 N4	G31 O6	14.46%	LT7 N3	A25 N1	22.30%
LG6 N2	C26 O2	14.22%	DT4 N3	A28 N1	13.64%	LG6 N1	C26 N3	20.66%
LT7 N3	A25 N1	14.16%	DA11 N6	U21 O4	13.56%	LA3 N6	U29 O4	18.46%
LC14 O2	G17 N2	12.72%	LT7 O4	A25 N6	13.26%	DT13 O4	A19 N6	17.88%
LC12 N4	G20 O6	12.36%	LC14 O2	G18 N1	12.40%	LT7 O4	A25 N6	16.20%
DA11 N6	U21 O4	11.34%	LC12 N3	G20 N2	11.76%	DT13 N3	A19 N1	15.78%
LC14 N3	G18 N1	11.22%	LC15 O2	G17 N2	11.40%	LG6 N1	C26 O2	15.44%
LC14 N3	G17 N1	10.96%	DT13 O2	A19 N6	10.70%	LA3 N1	U29 N3	11.18%
DT5 N3	A27 N1	10.38%	LC14 O2	G18 N2	10.16%	DT5 N3	A27 N1	10.46%
LG6 N1	C26 N3	10.08%	LC12 N3	G20 N1	10.16%			

HDO-antimiR 1			HDO-antimiR 2			HDO-antimiR 3		
HDO	miRNA	freq.	HDO	miRNA	freq.	HDO	miRNA	freq.
A24 N6	U38 O4	28.70%	LC1 N4	G45 O6	45.66%	A27 O2'	A42 N3	29.50%
A18 OP2	G32 N2	28.30%	DC2 N4	U44 O4	45.62%	G17 OP2	U31 N3	23.12%
A24 N7	G39 N2	20.00%	A24 N6	U38 O4	37.38%	LG6 O6	G39 N1	19.76%
LT7 O2	G37 N1	19.84%	G30 O6	U44 N3	29.36%	G21 N7	G35 N2	19.74%
G21 O6	G35 N2	18.94%	DT5 O4	A40 N6	27.68%	A26 N6	A40 N3	16.86%
G23 N7	G37 N2	17.26%	U22 O4	G37 N2	24.30%	DT5 O4	A40 N6	15.84%
LA3 N6	A42 N1	11.48%	LG6 O6	G39 N1	22.92%	LA3 N1	C41 N4	15.84%
G19 OP2	G33 N2	11.12%	DC2 O2	G46 N2	21.32%	G16 N7	U31 O5'	14.54%
DC2 N4	A43 N1	10.04%	A18 N7	G33 N2	19.56%	DC2 O2	G46 N2	13.26%
			A27 N6	A42 N1	18.92%	LG6 N1	G39 N2	12.74%
			A24 N7	G39 N2	18.00%	A24 N6	U38 O4	12.22%
			A26 N6	A40 O2'	17.58%	G21 O6	G35 N1	11.30%
			LC1 O2	G46 N1	16.14%	G17 OP2	G32 N2	10.26%
			U20 O4	G35 N2	15.12%	G23 O6	G37 N2	10.26%
			LA3 N6	C41 N3	14.52%	G29 O6	A42 N6	10.12%
			G23 O6	G37 N2	14.22%			
			DT4 O4	C41 N4	13.98%			

The frequency of the binding site of the antimiR122 or HDO-antimiR122 with miR122 when along the Z axis -5 Å (more than 10% frequency)

Supplementary Table 5

antimiR 1			antimiR 2			antimiR 3		
antimiR	miRNA	freq.	antimiR	miRNA	freq.	antimiR	miRNA	freq.
DC2 O2	G30 N2	48.68%	DC2 O2	G30 N2	53.34%	LC6 O2	G26 N2	43.30%
LC6 O2	G26 N2	43.88%	DG8 N2	C24 O2	49.76%	DG8 N2	C24 O2	42.96%
LA12 N6	U20 O4	42.08%	DG13 N2	C19 O2	43.32%	DG13 N2	C19 O2	42.68%
DG4 N2	C28 O2	41.78%	LC6 O2	G26 N2	40.98%	DC2 O2	G30 N2	42.30%
DG13 N2	C19 O2	41.52%	DG8 O6	C24 N4	40.46%	LA12 N6	U20 O4	38.22%
LC14 O2	G18 N2	41.12%	DG8 N1	C24 N3	40.22%	DA9 N6	U23 O4	34.52%
DG8 N2	C24 O2	40.58%	LA3 N6	U29 O4	39.76%	DG8 O6	C24 N4	33.66%
DG4 O6	C28 N4	39.88%	DA9 N6	U23 O4	39.36%	DC2 N4	G30 O6	33.36%
LC6 N3	G26 N1	39.58%	DG4 N2	C28 O2	37.48%	LT10 O4	A22 N6	33.00%
DG4 N1	C28 N3	38.24%	DC2 N3	G30 N1	36.70%	DG8 N1	C24 N3	33.00%
DA11 N6	U21 O4	37.64%	LC14 O2	G18 N2	36.22%	LC14 O2	G18 N2	32.26%
LT10 O4	A22 N6	37.28%	LT7 O4	A25 N6	35.58%	LC6 N3	G26 N1	31.70%
DC2 N3	G30 N1	35.72%	LA12 N6	U20 O4	35.52%	DG13 N1	C19 N3	31.50%
DC2 N4	G30 O6	34.40%	DG4 O6	C28 N4	34.50%	LT7 O4	A25 N6	31.16%
LA3 N6	U29 O4	34.40%	DG4 N1	C28 N3	32.28%	DA11 N6	U21 O4	30.98%
DG13 O6	C19 N4	32.44%	DG13 O6	C19 N4	31.80%	DG13 O6	C19 N4	30.94%
LC14 N3	G18 N1	31.16%	DG13 N1	C19 N3	30.92%	LC14 N3	G18 N1	27.86%
LC6 N4	G26 O6	30.00%	LC14 N3	G18 N1	30.80%	DA11 N1	U21 N3	26.78%
DG8 O6	C24 N4	29.88%	DA11 N6	U21 O4	30.60%	DC2 N3	G30 N1	26.60%
DG13 N1	C19 N3	28.74%	DC2 N4	G30 O6	29.90%	LT15 O4	A17 N6	26.02%
DG8 N1	C24 N3	26.18%	LT10 O4	A22 N6	28.90%	LC14 N4	G18 O6	25.96%
LT7 O4	A25 N6	26.06%	LC6 N3	G26 N1	27.66%	DA9 N1	U23 N3	23.66%
DT5 O4	A27 N6	26.04%	LC14 N4	G18 O6	24.20%	LC6 N4	G26 O6	20.60%
DA11 N1	U21 N3	25.92%	DT5 O4	A27 N6	23.78%	LT10 N3	A22 N1	19.32%
LC14 N4	G18 O6	24.42%	LT10 N3	A22 N1	21.16%	DT5 O4	A27 N6	18.18%
LA3 N1	U29 N3	23.14%	DA11 N1	U21 N3	20.44%	LA12 N1	U20 N3	17.18%
LT1 O4	A31 N6	18.32%	LA3 N1	U29 N3	17.98%	LT7 N3	A25 N1	16.90%
LT7 N3	A25 N1	17.82%	LT7 N3	A25 N1	17.94%	DG4 N2	C28 O2	16.38%
LT1 O4'	G33 N2	16.68%	LC6 N4	G26 O6	16.60%	DG4 O6	C28 N4	15.14%
DT5 N3	A27 N1	14.54%	LA12 N1	U20 N3	16.08%	LT1 O4	A31 N6	15.06%
LA12 N1	U20 N3	13.28%	LT15 O4	A17 N6	15.52%	LT15 N3	A17 N1	11.90%
LT1 O5'	G33 N3	10.36%	DT5 N3	A27 N1	15.04%	LA3 N6	U29 O2	11.18%
			DC2 O2	A31 N6	13.54%	LA3 N6	C28 O2	10.30%
			LA3 O4'	A31 N6	13.22%			
			DC2 O2	U32 N3	11.40%			
			DA9 N1	U23 N3	10.26%			

HDO-antimiR 1			HDO-antimiR 2			HDO-antimiR 3		
HDO	miRNA	freq.	HDO	miRNA	freq.	HDO	miRNA	freq.
A21 N6	U35 O4	38.32%	C27 N4	A42 O2'	37.72%	LT1 O2'	A42 N6	13.90%
C27 N4	A42 O2'	31.26%	LA12 N6	G33 O6	30.82%	DG4 O6	G41 N1	13.30%
C18 N4	A32 N1	26.68%	G29 N7	C43 O2'	22.68%	A21 N6	U36 O4	12.94%
U20 O4	C34 N4	22.46%	A21 N6	U36 O4	21.44%	G29 O6	C43 N4	10.46%
G17 O6	U31 N3	20.12%	DG4 O6	G41 N1	20.02%	A24 N6	U38 O4	10.14%
C23 N4	A37 N1	16.38%	A24 OP2	C39 N4	19.86%			
A21 N7	U35 N3	14.92%	DG8 O6	A37 N6	19.54%			
DG4 O6	G41 N1	12.70%	U20 O4	G33 N2	18.96%			
A24 N6	U38 O4	11.86%	LA3 N6	G41 O6	17.98%			
A16 O5'	G33 OP1	10.32%	C23 N4	U36 O2'	14.28%			
			LA12 N1	G33 N1	14.24%			
			U20 O4	C34 N4	12.80%			
			A30 N1	G45 N2	11.82%			
			C18 N4	A32 N1	10.40%			

The frequency of the binding site of the antimiR21 or HDO-antimiR21 with miR21 when along the Z axis -5 Å.
(more than 10% frequency)